Simulating Propagation of High Harmonic Generation in Bulk Solids

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High harmonic generation (HHG) in solids is an emerging area of extreme nonlinear optics with applications in ultrafast spectroscopy, metrology, and the study of novel quantum materials. Only a few previous studies, however, account for propagation through the bulk material, leaving open questions about the underlying mechanism. Specifically, unphysically short dephasing times are required in simulation to reproduce the distinct harmonic peaks of experimental HHG spectra, and recent studies attribute this discrepancy to overlooked interactions with the bulk material. We simulate propagation of high-order harmonics in bulk GaAs and Sapphire by a high-intensity terahertz driving pulse in order to compare propagation effects in semiconducting and insulating materials. The interband polarization response is calculated by the semiconductor Bloch equations (SBEs), and material properties are calculated using density functional theory implemented in the Vienna Ab-initio Simulation Package (VASP). The SBEs are coupled to a unidirectional pulse propagation equation through integration with open-source software Lightwave Explorer. The resulting insights into HHG propagation through bulk solids are prerequisite to connecting the output spectra to the underlying microscopic mechanism and thereby essential to building more accurate predictive models of solid HHG in order to facilitate material engineering control of attosecond HHG pulses.

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